

Chemistry Report for Case # P-18-0136

General

Submitter: [REDACTED].

Contact: [REDACTED]

Contact Telephone No.: [REDACTED]

TS No.: MKP100

Chemist: Yakal, Randy

Contractor Support: Y

PV Init (kg/yr): [REDACTED]

PV Max (kg/yr): [REDACTED]

Binding Option: ☐

Exposure-Based Review: [REDACTED]

Manufacture: ☐

Import: ☒

CAS Number: [REDACTED]

Chemical Name [REDACTED]
[REDACTED]
[REDACTED]
[REDACTED]

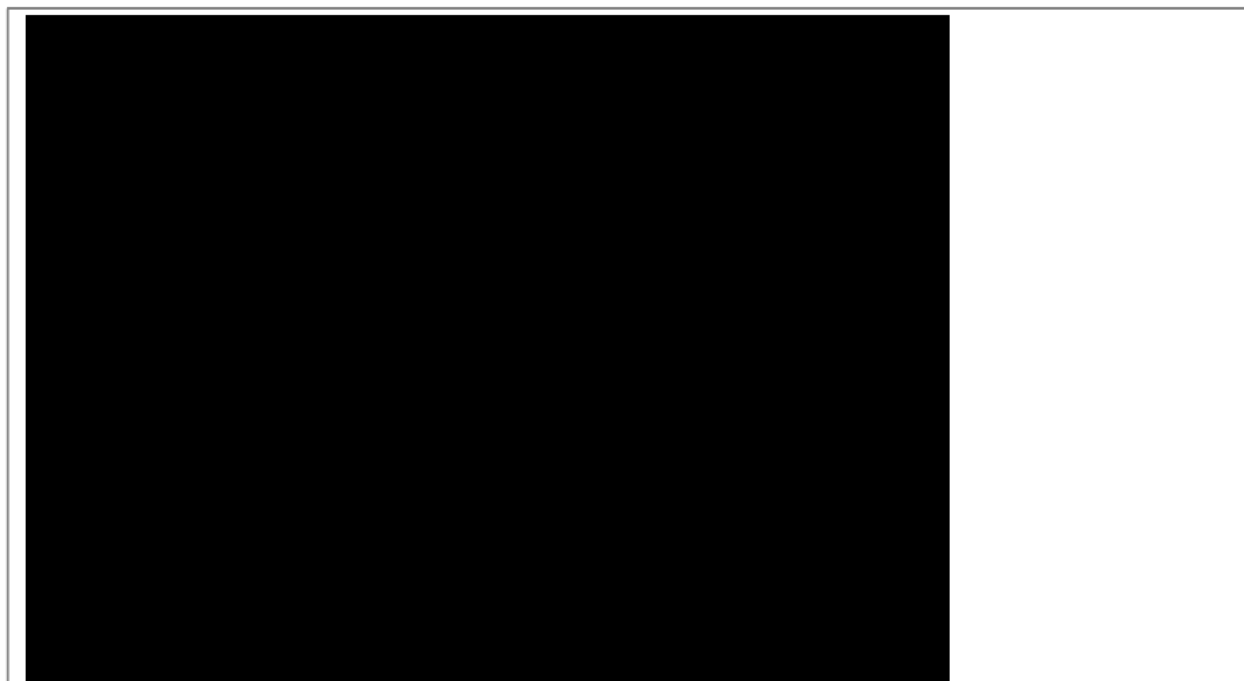
Trade Name: MKP 1003

IES Order: 427922

Generic Name: 1-Butanaminium,
N,N,N-tributyl-,
2(or5)-[[benzoyldihydrodioxo[(sulfophenyl)amino]heteropolycycle]oxy]-5(or
2)-(1,1-dimethylpropyl)benzenesulfonate (2:1)

Chemical Structure





Physical Chemical Properties

Molecular Formula: [REDACTED]	Molecular Weight: [REDACTED]
[REDACTED]	
% < 500:	% < 1000:
MP:	MP Estimate:
BP:	BP Pressure:
BP Estimate:	
VP (Torr):	VP Estimate (Torr): <0.000001
Water Solubility (g/L): 2.067	Water Soluble Estimate (g/L):
Log P: 1.74	Log P Estimate:
Physical State — Neat: Solid	Physical State — Manuf: NK - Imported in formulation

Physical State — Processing: Solid, [REDACTED] PMN material in [REDACTED]

Physical State — End Use: Solid, PMN material [REDACTED]

Additional Chemical Info

Submitted

data: magenta solid; VP = 3.5E-8 torr at 23 °C; WS = 2.067 g/L (OECD 105); log P = 1.739 (OECD 107); density = 1.15 g/cc (OECD 109); surface tension = 52.2 nM.m-1 (OECD 115, ring method); not flammable.

SMILES for the anion as a free acid:

[REDACTED]

SMILES

for the cation as a chloride salt:

[REDACTED]

Uses

Consumer Use? No

Use:

[REDACTED] The anion portion of the PMN material is [REDACTED]
All analogs are dyes for [REDACTED]

Other Uses:

No other uses were found for the PMN material.

Reaction Description

The PMN material is imported. The proposed synthesis is based on the description given on page 4a of the submission. [REDACTED]

[REDACTED]

Pollution Prevention Analysis(P2 Analysis:)

No

Pollution Prevention information was provided by the submitter.

Analogs

[REDACTED]

Analogs: [REDACTED]

Comments/Telephone Log

Artifact	Update/Upload Time
[REDACTED]	[REDACTED]